

10/576,335

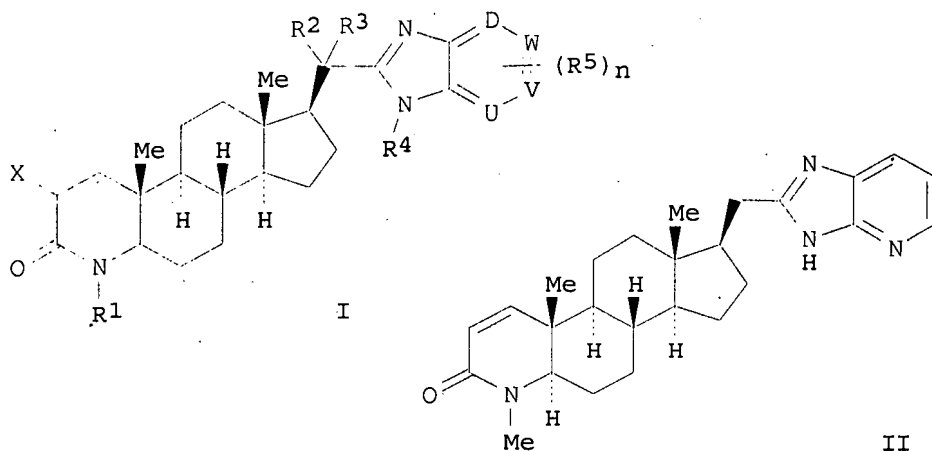
STM- Structure Search
8/6/07

=> d ibib abs hitstr

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
 INVENTOR(S):
 ACCESSION NUMBER: 2005:429530 CAPLUS
 DOCUMENT NUMBER: 142:482188
 TITLE: Preparation of 21-heterocyclic-4-azasteroid derivatives as selective androgen receptor modulators
 INVENTOR(S): Dankulich, William P.; Mitchell, Helen J.
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA
 SOURCE: PCT Int. Appl., 85 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005044988	A2	20050519	WO 2004-US35838	20041027
WO 2005044988	A3	20051027		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004288196	A1	20050519	AU 2004-288196	20041027
CA 2543956	A1	20050519	CA 2004-2543956	20041027
EP 1696925	A2	20060906	EP 2004-796663	20041027
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1871005	A	20061129	CN 2004-80031558	20041027
JP 2007509962	T	20070419	JP 2006-538255	20041027
IN 2006DN01930	A	20070615	IN 2006-DN1930	20060407
US 2007088047	A1	20070419	US 2006-576335	20060418
PRIORITY APPLN. INFO.:				
			US 2003-516425P	P 20031031
			WO 2004-US35838	W 20041027

OTHER SOURCE(S): MARPAT 142:482188
 GI



AB Azasteroids of formula I [X = H, halo; R1 = H, CF3, acyl, alkyl, etc.; R2, R3 = H, halo, alkyl, aminoalkyl, etc.; R2R3 = oxo, alkylene; R4 = H, halo, acyl, arylalkyl, etc.; R5 = H, acyl, alkoxycarbonylalkyl, etc.; U, V, W, D = CH, N, with provisos] are prepared as modulators of the androgen receptor (AR) in a tissue selective manner. They are useful as agonists of the androgen receptor in bone and/or muscle tissue while antagonizing the AR in the prostate of a male patient or in the uterus of a female patient. These compds. are therefore useful in the enhancement of weakened muscle tone and the treatment of conditions caused by androgen deficiency or which can be ameliorated by androgen administration, including osteoporosis, osteopenia, glucocorticoid-induced osteoporosis, periodontal disease, bone fracture, bone damage following bone reconstructive surgery, sarcopenia, frailty, aging skin, male hypogonadism, postmenopausal symptoms in women, atherosclerosis, hypercholesterolemia, hyperlipidemia, obesity, aplastic anemia and other hematopoietic disorders, inflammatory arthritis and joint repair, HIV-wasting, prostate cancer, cancer cachexia, Alzheimer's disease, muscular dystrophies, cognitive impairment, decreased libido, premature ovarian failure, and autoimmune disease, alone or in combination with other active agents. Thus, II was prepared in several steps from 4-methyl-3-oxo-4-aza-5 α -androst-1-ene-17 β -carboxylic acid and 2,3-diaminopyridine. The prepared compds. had IC50 values of 1 μ M or less in hydroxylapatite-based radioligand displacement assay.

IT 851866-03-0P

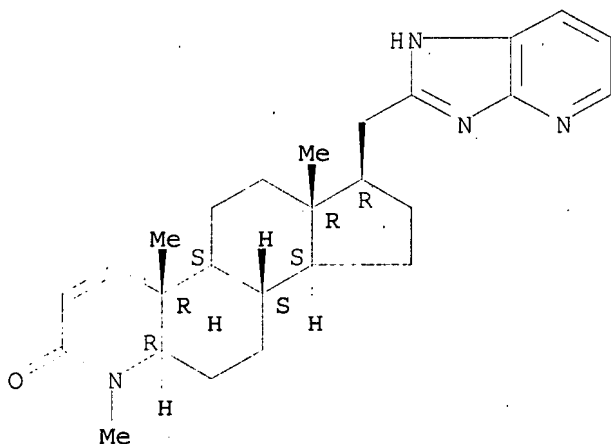
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of heterocyclic azasteroid derivs. as selective androgen receptor modulators)

RN 851866-03-0 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-7-(1H-imidazo[4,5-b]pyridin-2-ylmethyl)-1,4a,6a-trimethyl-, (4aR,4bS,6aR,7R,9aS,9bS,11aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 851866-04-1P 851866-05-2P 851866-06-3P
 851866-07-4P 851866-08-5P 851866-09-6P
 851866-10-9P 851866-11-0P 851866-12-1P
 851866-13-2P 851866-14-3P 851866-15-4P
 851866-16-5P 851866-17-6P 851866-18-7P
 851866-19-8P 851866-20-1P 851866-21-2P
 851866-22-3P 851866-23-4P 851866-24-5P
 851866-25-6P 851866-26-7P 851866-27-8P

10/576,335

851866-28-9P 851866-29-0P 851866-30-3P
851866-31-4P 851866-32-5P 851866-33-6P
851866-34-7P 851866-35-8P 851866-36-9P
851866-37-0P

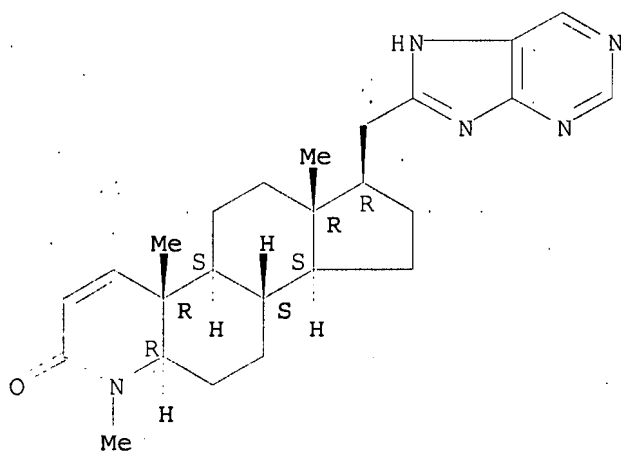
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic azasteroid derivs. as selective androgen receptor modulators)

RN 851866-04-1 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-7-(1H-purin-8-ylmethyl)-, (4aR,4bS,6aR,7R,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

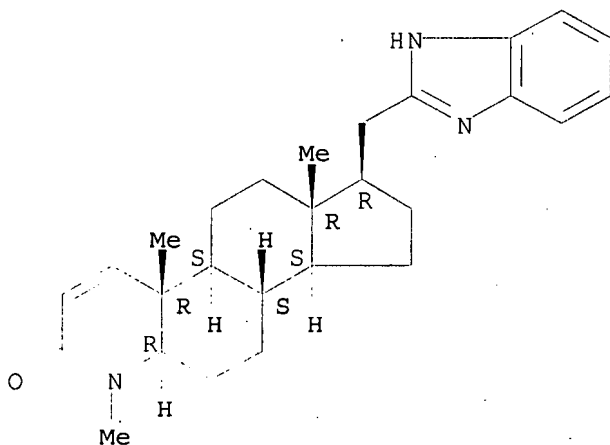
Absolute stereochemistry.



RN 851866-05-2 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 7-(1H-benzimidazol-2-ylmethyl)-1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-, (4aR,4bS,6aR,7R,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

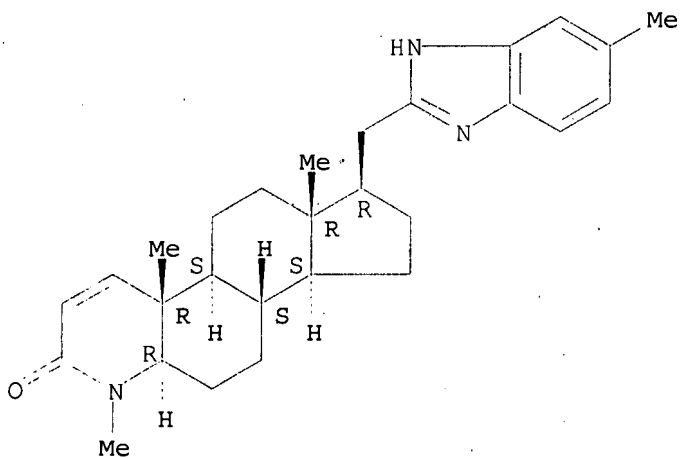
Absolute stereochemistry.



RN 851866-06-3 CAPLUS

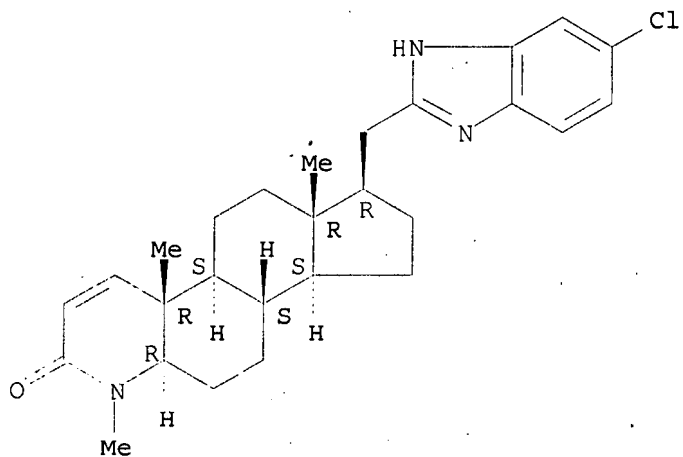
CN 2H-Indeno[5,4-f]quinolin-2-one, 1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-7-[(5-methyl-1H-benzimidazol-2-yl)methyl]-, (4aR,4bS,6aR,7R,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CN 2H-Indeno[5,4-f]quinolin-2-one, 7-[(5-chloro-1H-benzimidazol-2-yl)methyl]-
1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-,
(4aR,4bS,6aR,7R,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

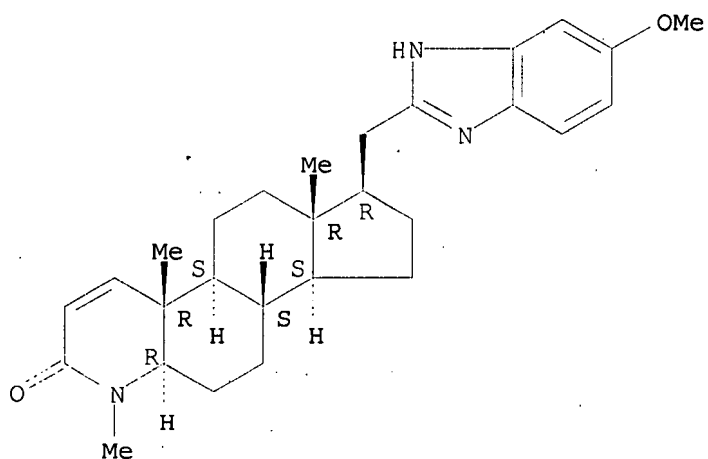
Absolute stereochemistry.



CN 2H-Indeno[5,4-f]quinolin-2-one, 1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-7-[(5-methoxy-1H-benzimidazol-2-yl)methyl]-1,4a,6a-trimethyl-, (4aR,4bS,6aR,7R,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

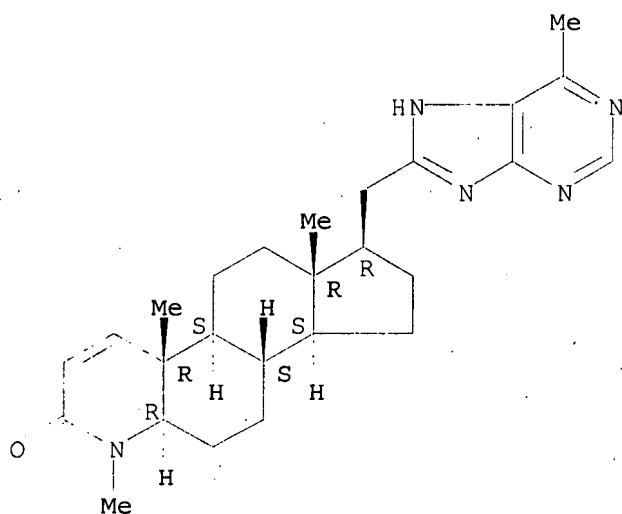
10/576,335



RN 851866-09-6 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-7-[(6-methyl-1H-purin-8-yl)methyl]-, (4aR,4bS,6aR,7R,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

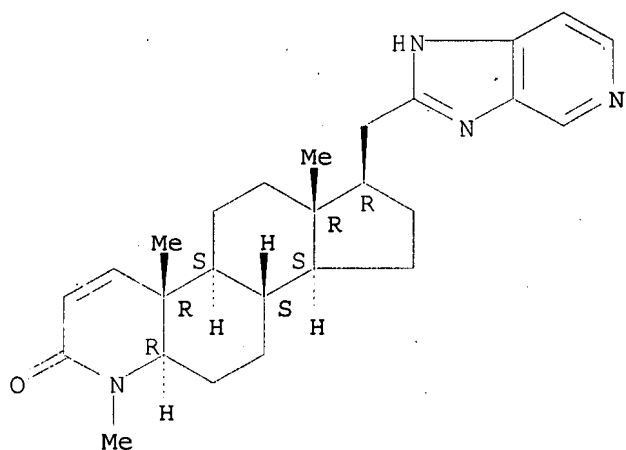
Absolute stereochemistry.



RN 851866-10-9 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-7-(1H-imidazo[4,5-c]pyridin-2-ylmethyl)-1,4a,6a-trimethyl-, (4aR,4bS,6aR,7R,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

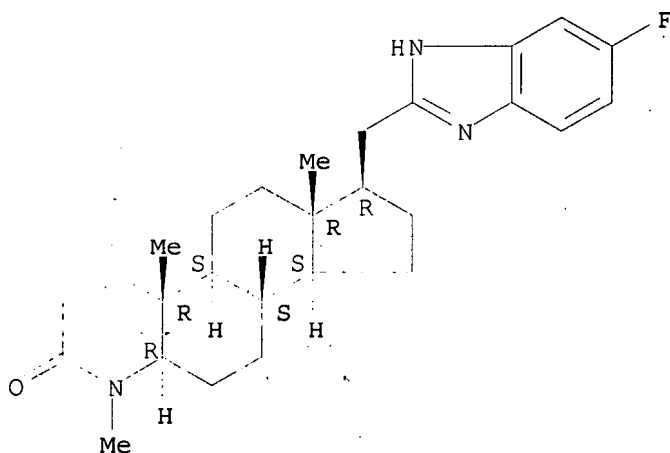
Absolute stereochemistry.



RN 851866-11-0 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 7-[(5-fluoro-1H-benzimidazol-2-yl)methyl]-
1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-,
(4aR,4bS,6aR,7R,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

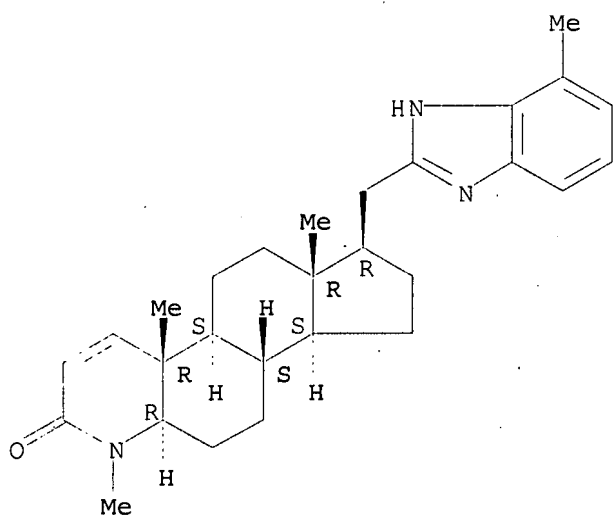


RN 851866-12-1 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-
tetradecahydro-1,4a,6a-trimethyl-7-[(4-methyl-1H-benzimidazol-2-yl)methyl]-
, (4aR,4bS,6aR,7R,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

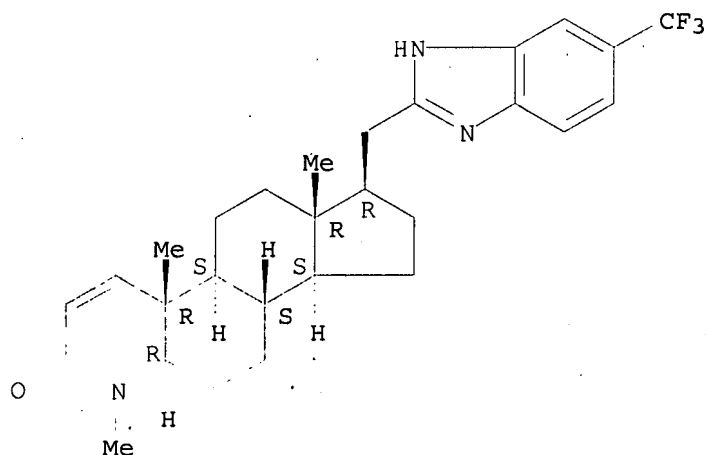
Absolute stereochemistry.

10/576,335



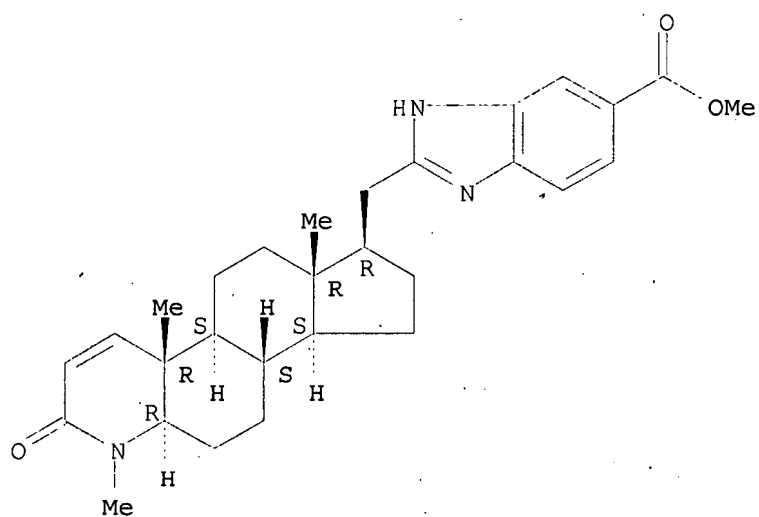
RN 851866-13-2 CAPLUS
 CN 2H-Indeno[5,4-f]quinolin-2-one, 1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-7-[[5-(trifluoromethyl)-1H-benzimidazol-2-yl]methyl]-, (4aR,4bS,6aR,7R,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 851866-14-3 CAPLUS
 CN 1H-Benzimidazole-5-carboxylic acid, 2-[[[(4aR,4bS,6aR,7R,9aS,9bS,11aR)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

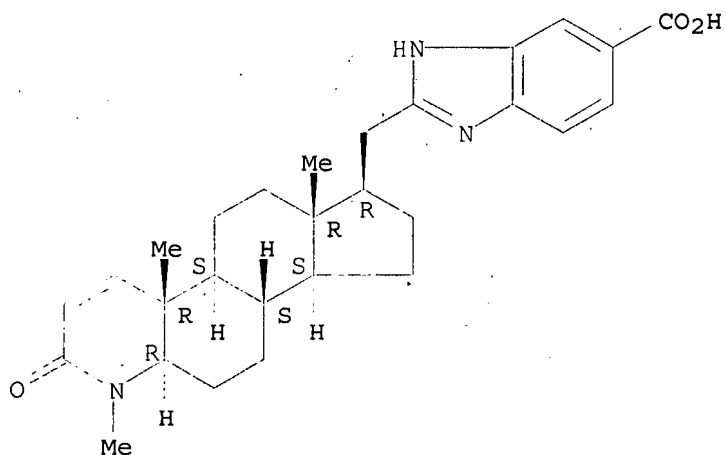
Absolute stereochemistry.



RN 851866-15-4 CAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[[[(4aR,4bS,6aR,7R,9aS,9bS,11aR)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-yl)methyl]- (9CI) (CA INDEX NAME)

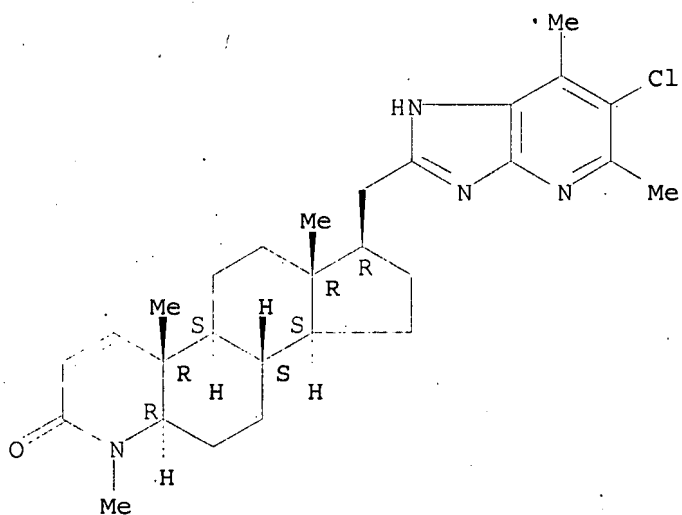
Absolute stereochemistry.



RN 851866-16-5 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 7-[[[(6-chloro-5,7-dimethyl-1H-imidazo[4,5-b]pyridin-2-yl)methyl]-1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-, (4aR,4bS,6aR,7R,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

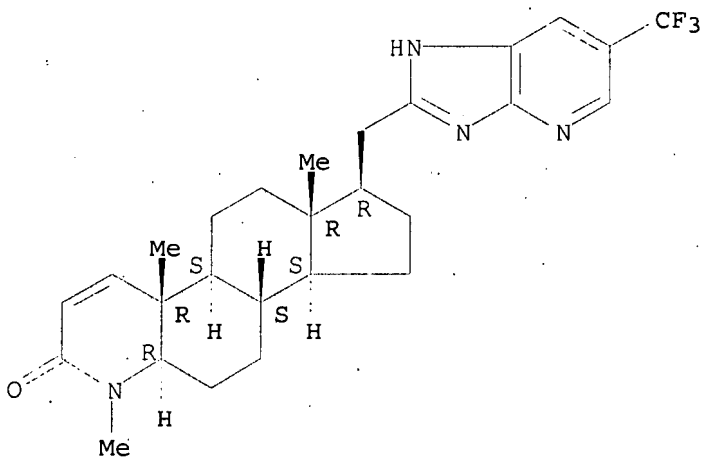
Absolute stereochemistry.



RN 851866-17-6 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-7-[[6-(trifluoromethyl)-1H-imidazo[4,5-b]pyridin-2-yl]methyl]-, (4aR,4bS,6aR,7R,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

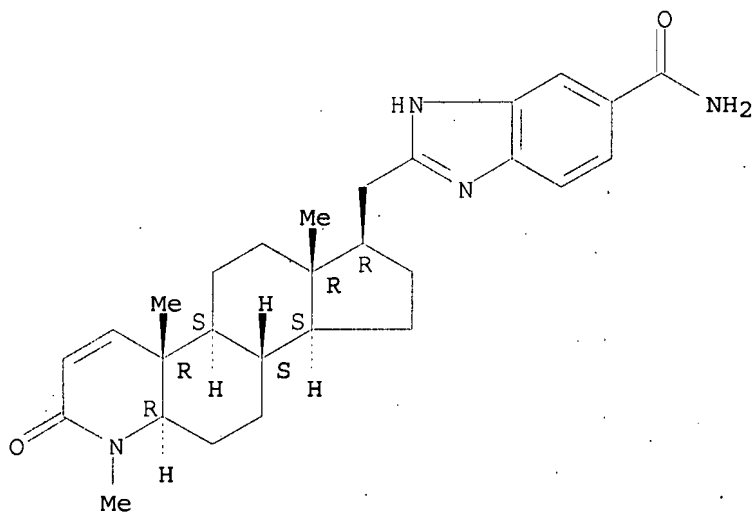
Absolute stereochemistry.



RN 851866-18-7 CAPLUS

CN 1H-Benzimidazole-5-carboxamide, 2-[[[(4aR,4bS,6aR,7R,9aS,9bS,11aR)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-yl]methyl]- (9CI) (CA INDEX NAME)

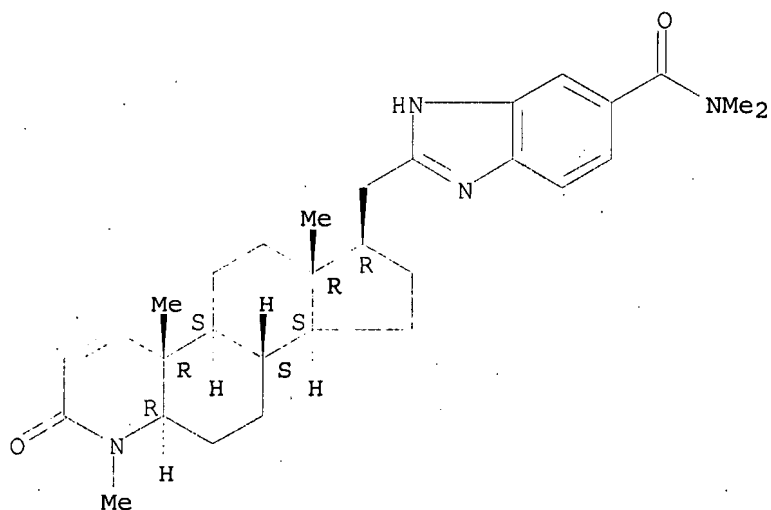
Absolute stereochemistry.



RN 851866-19-8 CAPLUS

CN 1H-Benzimidazole-5-carboxamide, N,N-dimethyl-2-
[[[(4aR,4bS,6aR,7R,9aS,9bS,11aR)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-
tetradecahydro-1,4a,6a-trimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-
yl)methyl]]- (9CI) (CA INDEX NAME)

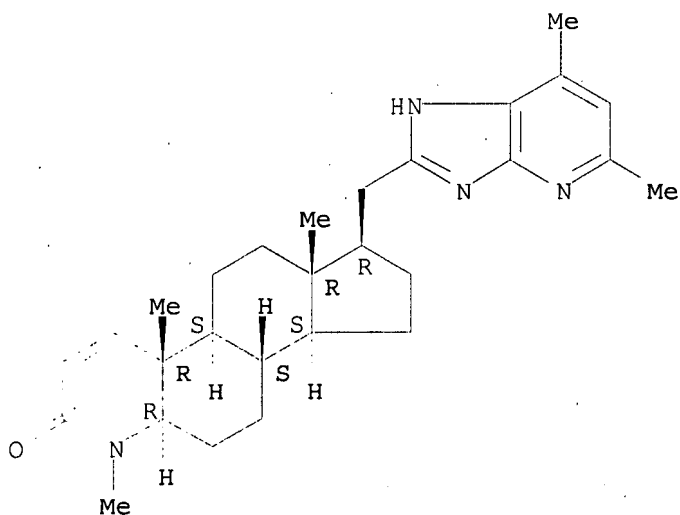
Absolute stereochemistry.



RN 851866-20-1 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 7-[(5,7-dimethyl-1H-imidazo[4,5-b]pyridin-
2-yl)methyl]-1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-
trimethyl-, (4aR,4bS,6aR,7R,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

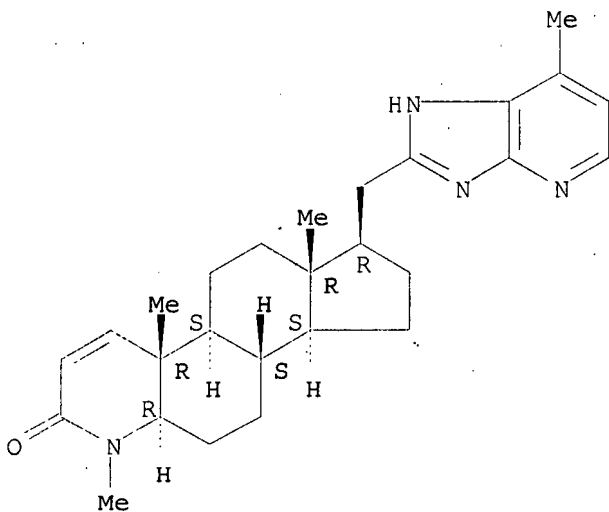
Absolute stereochemistry.



RN 851866-21-2 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-7-[(7-methyl-1H-imidazo[4,5-b]pyridin-2-yl)methyl]-, (4aR,4bS,6aR,7R,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

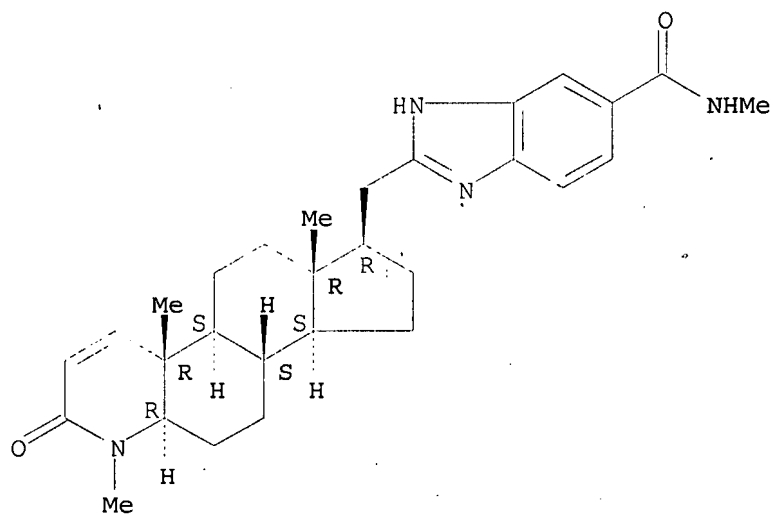
Absolute stereochemistry.



RN 851866-22-3 CAPLUS

CN 1H-Benzimidazole-5-carboxamide, N-methyl-2-[[[(4aR,4bS,6aR,7R,9aS,9bS,11aR)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-yl)methyl]- (9CI) (CA INDEX NAME)

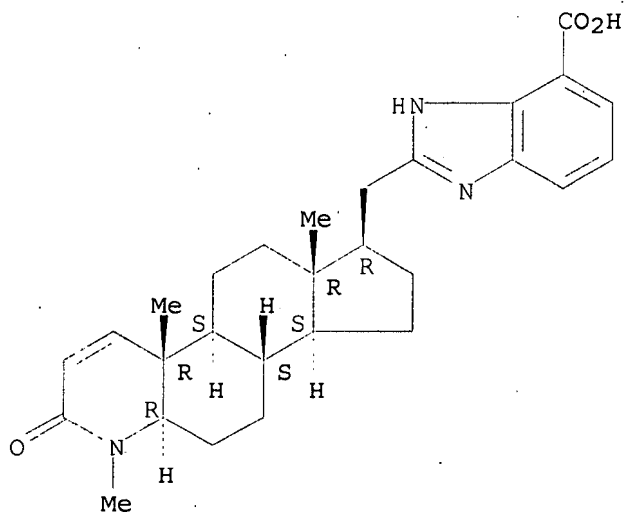
Absolute stereochemistry.



RN 851866-23-4 CAPLUS

CN 1H-Benzimidazole-4-carboxylic acid, 2-[[[(4aR,4bS,6aR,7R,9aS,9bS,11aR)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-yl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

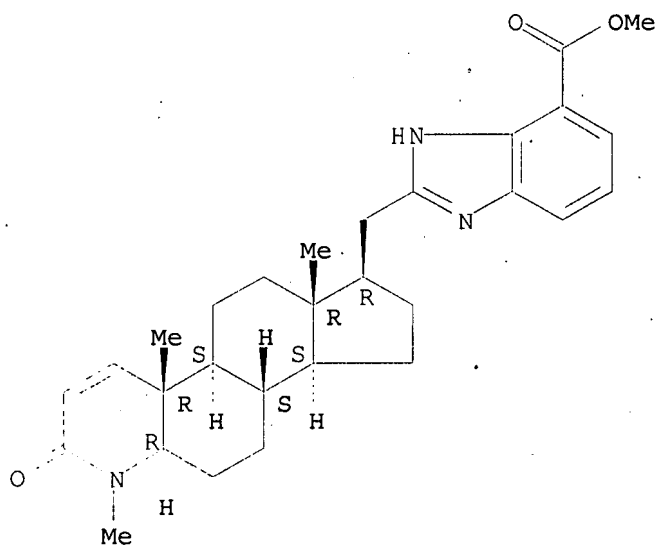


RN 851866-24-5 CAPLUS

CN 1H-Benzimidazole-4-carboxylic acid, 2-[[[(4aR,4bS,6aR,7R,9aS,9bS,11aR)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

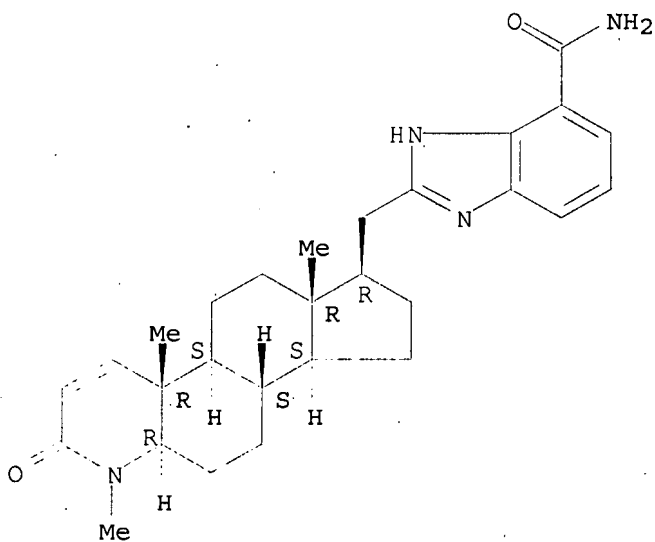
10/576,335



RN 851866-25-6 CAPLUS

CN 1H-Benzimidazole-4-carboxamide, 2-[[[(4aR,4bS,6aR,7R,9aS,9bS,11aR)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-yl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

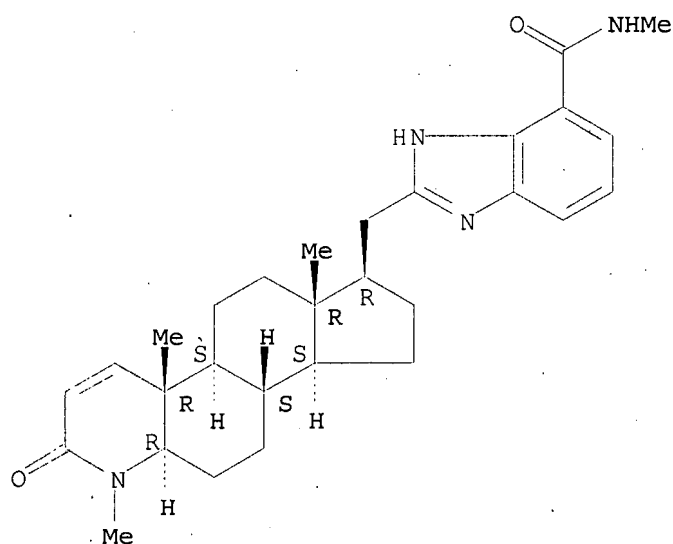


RN 851866-26-7 CAPLUS

CN 1H-Benzimidazole-4-carboxamide, N-methyl-2-[[[(4aR,4bS,6aR,7R,9aS,9bS,11aR)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-yl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

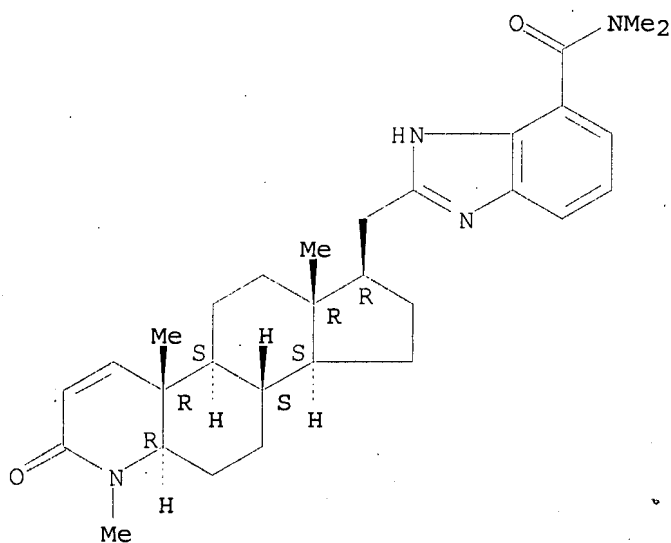
10/576,335



RN 851866-27-8 CAPLUS

CN 1H-Benzimidazole-4-carboxamide, N,N-dimethyl-2-
[[(4aR,4bS,6aR,7R,9aS,9bS,11aR) -2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-
tetradecahydro-1,4a,6a-trimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-
yl)methyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

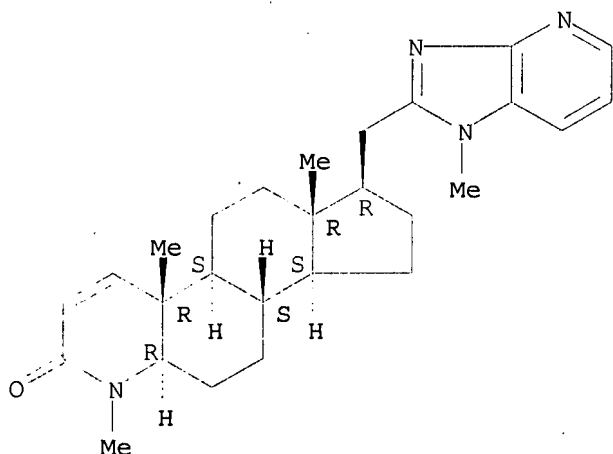


RN 851866-28-9 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-
tetradecahydro-1,4a,6a-trimethyl-7-[(1-methyl-1H-imidazo[4,5-b]pyridin-2-
yl)methyl] -, (4aR,4bS,6aR,7R,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

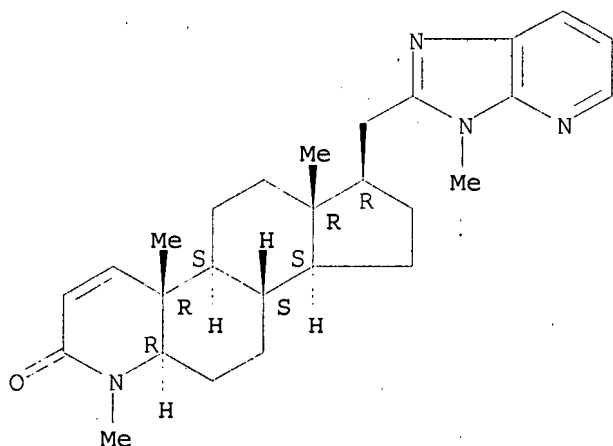
10/576,335



RN 851866-29-0 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-7-[(3-methyl-3H-imidazo[4,5-b]pyridin-2-yl)methyl]-, (4aR,4bS,6aR,7R,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

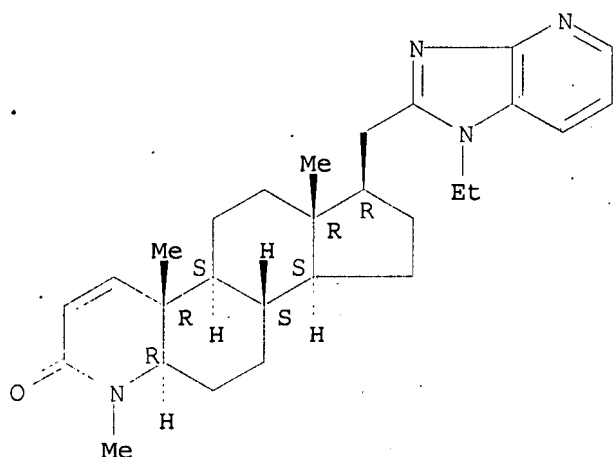
Absolute stereochemistry.



RN 851866-30-3 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 7-[(1-ethyl-1H-imidazo[4,5-b]pyridin-2-yl)methyl]-1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-, (4aR,4bS,6aR,7R,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

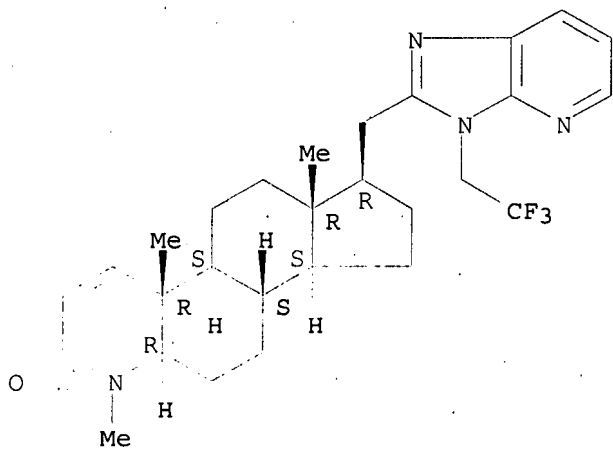
Absolute stereochemistry.



RN 851866-31-4 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-7-[[3-(2,2,2-trifluoroethyl)-3H-imidazo[4,5-b]pyridin-2-yl]methyl]-, (4aR,4bS,6aR,7R,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

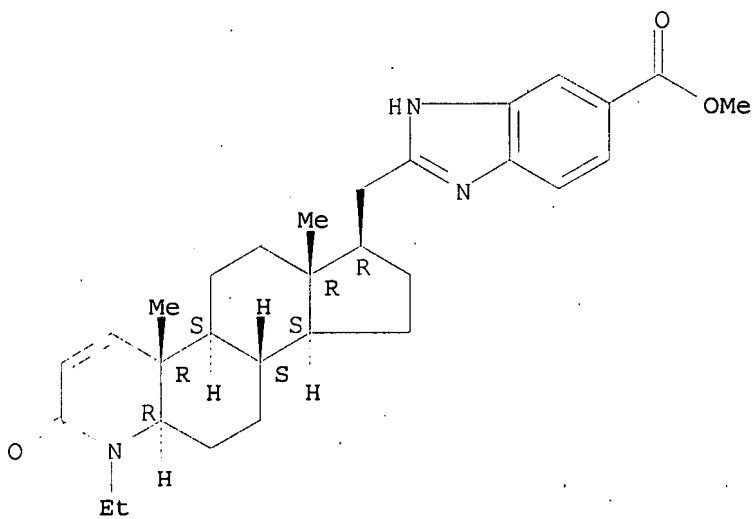


RN 851866-32-5 CAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[[[(4aR,4bS,6aR,7R,9aS,9bS,11aR)-1-ethyl-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

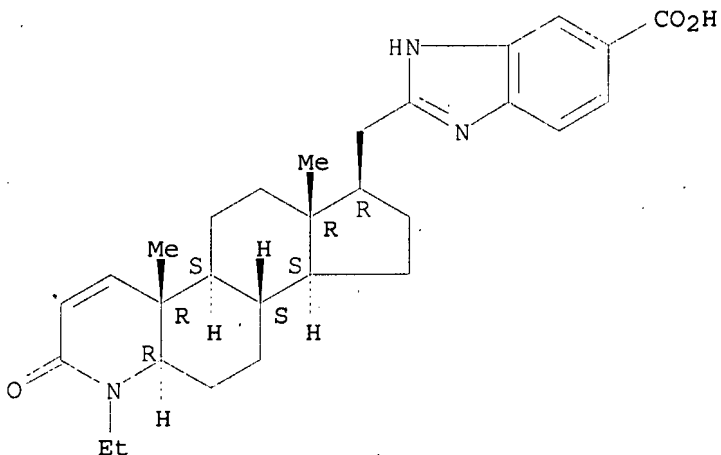
10/576,335



RN 851866-33-6 CAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[[[(4aR,4bS,6aR,7R,9aS,9bS,11aR)-1-ethyl-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-yl)methyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

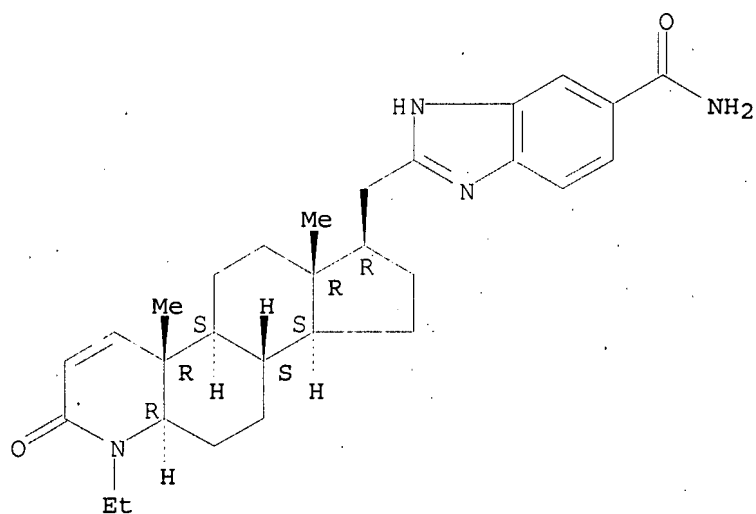


RN 851866-34-7 CAPLUS

CN 1H-Benzimidazole-5-carboxamide, 2-[[[(4aR,4bS,6aR,7R,9aS,9bS,11aR)-1-ethyl-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-yl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

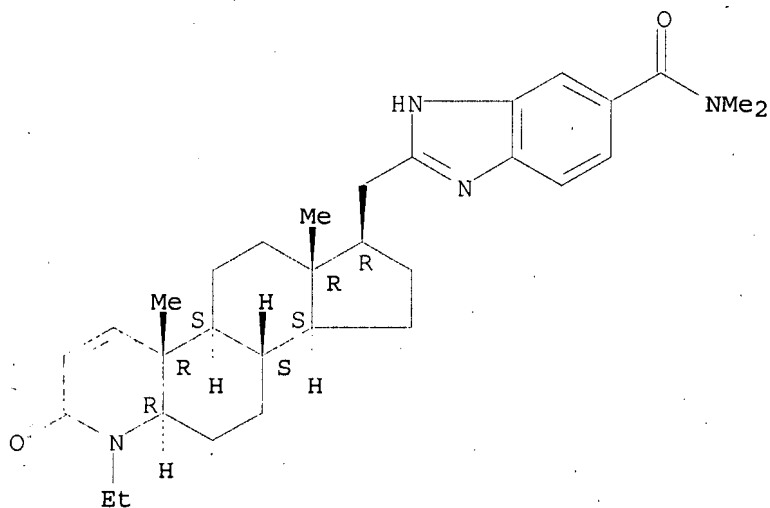
10/576,335



RN 851866-35-8 CAPLUS

CN 1H-Benzimidazole-5-carboxamide, 2-[[(4aR,4bS,6aR,7R,9aS,9bS,11aR)-1-ethyl-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-1H-indeno[5,4-f]quinolin-7-yl]methyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

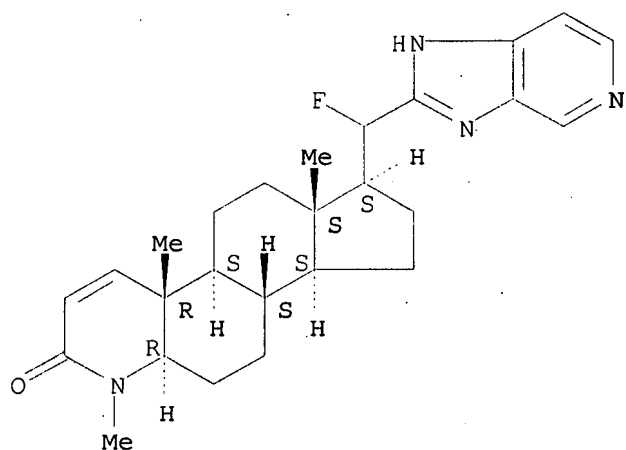


RN 851866-36-9 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 7-(fluoro-1H-imidazo[4,5-c]pyridin-2-ylmethyl)-1,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-1,4a,6a-trimethyl-, (4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

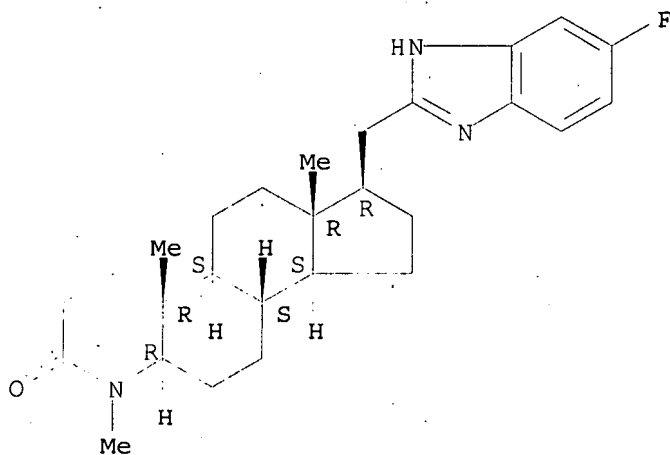
10/576,335



RN 851866-37-0 CAPLUS

CN 2H-Indeno[5,4-f]quinolin-2-one, 7-[(5-fluoro-1H-benzimidazol-2-yl)methyl]hexadecahydro-1,4a,6a-trimethyl-, (4aR,4bS,6aR,7R,9aS,9bS,11aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d his

(FILE 'HOME' ENTERED AT 11:18:12 ON 06 AUG 2007)

FILE 'REGISTRY' ENTERED AT 11:18:30 ON 06 AUG 2007

L1 STRUCTURE UPLOADED

L2 2 S L1

L3 35 S L1 FULL

FILE 'CAPLUS' ENTERED AT 11:19:28 ON 06 AUG 2007

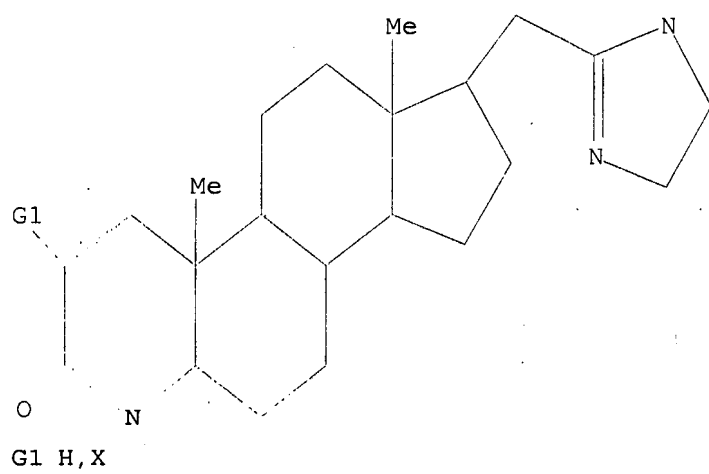
L4 1 S L3

=> d l1

L1 HAS NO ANSWERS

L1 STR

10/576,335



Structure attributes must be viewed using STN Express query preparation.

=>